SUPPLEMENTARY INFORMATION: Serpentine polymorphism: a quantitative insight from first-principle calculations.

Raffaella Demichelis,[1] Marco De La Pierre,[1] Mainak Mookherjee,[2]
Claudio M. Zicovich-Wilson,[3] and Roberto Orlando[4]

[1]*Nanochemistry Research Institute, Curtin Institute for Computation and Department of Chemistry, Curtin University, U1987, 6845 Perth, Western Australia, Australia*

[2]*Earth, Ocean and Atmospheric Sciences, Florida State University, Tallahassee, FL 32036, USA*

[3]*Centro de Investigación en Ciencias-(IICBA), Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, 62209 Cuernavaca, Morelos, Mexico*

[4]*Dipartimento di Chimica, Università degli Studi di Torino, Via Giuria 7, 10125 Torino, Italy*

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TABLE S1: File `Table_S1_ene.dat` contains data on the energy of single-walled $(n, -n)$ chrysotile nanotubes as a function of the index n. Data on the lizardite slab, units of measure and column titles can be found in the file header. Columns are numbered for easier handling when plotting.

TABLE S2: File `Table_S2_stru.dat` contains data on the structural parameters of single-walled $(n, -n)$ chrysotile nanotubes as a function of the index n. Data on the lizardite slab, units of measure and column titles can be found in the file header. Columns are numbered for easier handling when plotting.

TABLE S3: File `Table_S3_dist.dat` contains data on the atomic distances and angles of single-walled $(n, -n)$ chrysotile nanotubes as a function of the index n. Data on the lizardite slab, units of measure and column titles can be found in the file header. Columns are numbered for easier handling when plotting.

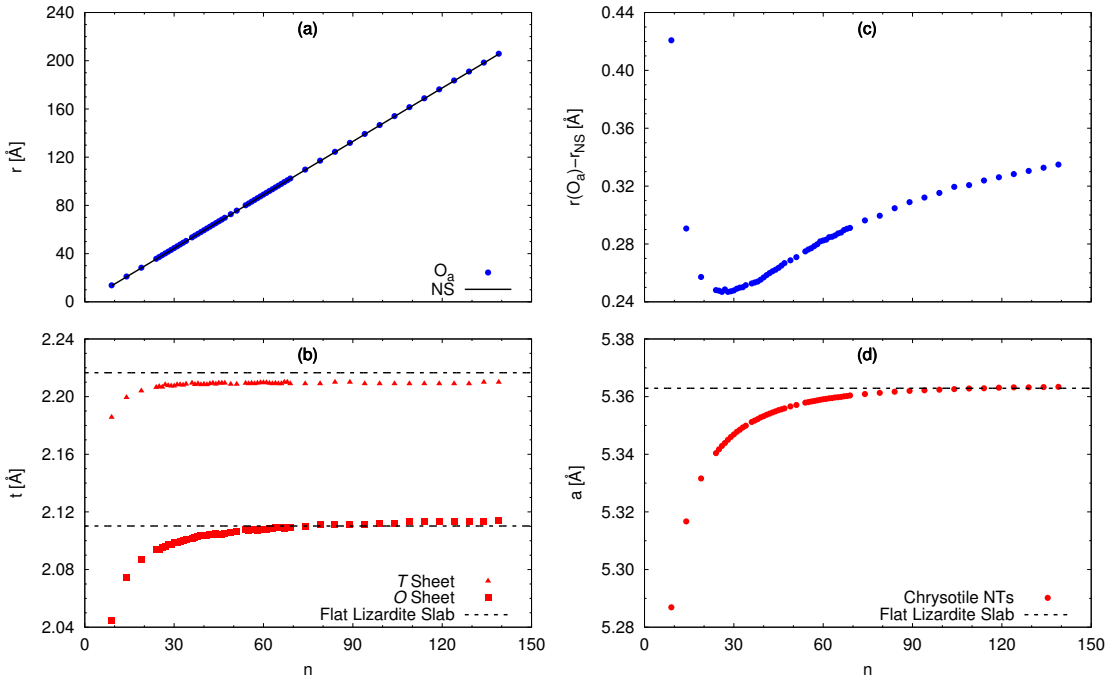

FIG. S1: Dependence of some structural parameters of single-walled $(n, -n)$ chrysotile nanotubes on the index n: (a) radius of O_a layer and of the NS; (b) thickness of the T and O sheets; (c) difference between O_a and NS radii; (d) lattice parameter. When defined, values for the flat lizardite slab are reported, too. All distances are in Å. The number of formula units and of atoms in the unit cell equals $2n$ and $36n$, respectively. The corresponding data are filed in Table S2 in the Supplementary Information.

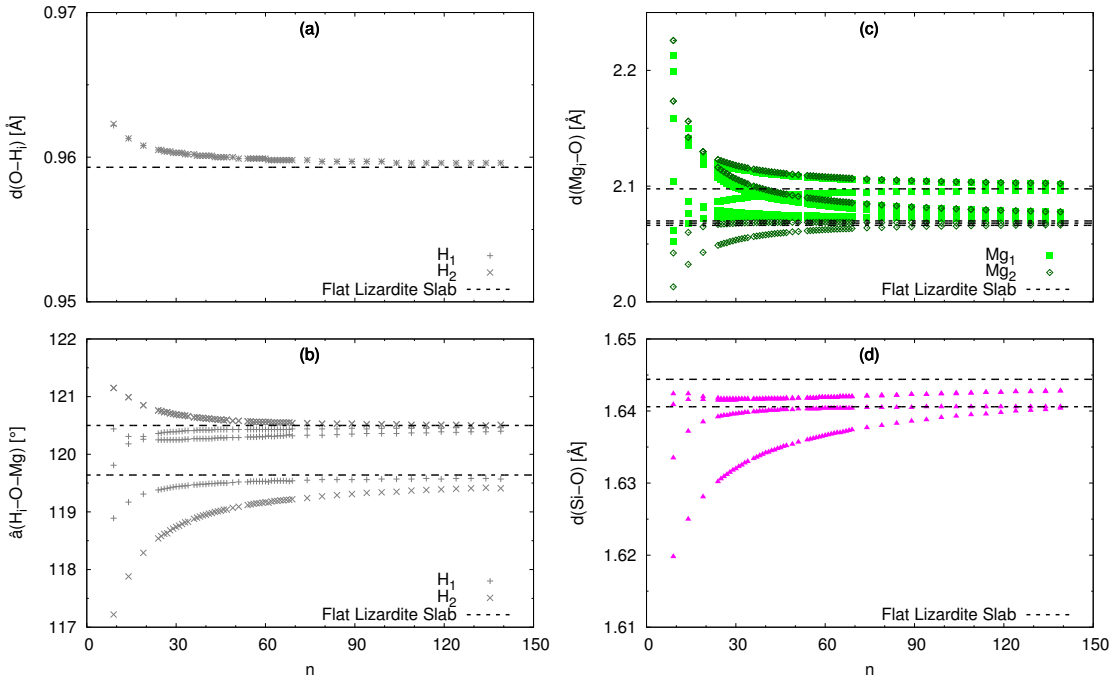

FIG. S2: Dependence of selected atomic distances and angles of single-walled $(n, -n)$ chrysotile nanotubes on the index n: (a) O-H distances for hydrogens on the outer surface; (b) H-O-Mg angles for hydrogens on the outer surface; (c) Mg-O distances; (d) Si-O distances. Values for the flat lizardite slab are reported, too. Distances are in Å, angles in degrees. Only symmetry independent atoms are considered. The corresponding data are filed in Table S3 in the Supplementary Information.